Connecting via Winsock to STN

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LOGINID:ssptatsh1654

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TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * * * * * * Welcome to STN International * * * * * * * * * *

NEWS 1		Web Page for STN Seminar Schedule - N. America
NEWS 2	AUG 15	CAOLD to be discontinued on December 31, 2008
NEWS 3	OCT 07	EPFULL enhanced with full implementation of EPC2000
NEWS 4	OCT 07	Multiple databases enhanced for more flexible patent number searching
NEWS 5	OCT 22	Current-awareness alert (SDI) setup and editing enhanced
NEWS 6	OCT 22	WPIDS, WPINDEX, and WPIX enhanced with Canadian PCT Applications
NEWS 7	OCT 24	CHEMLIST enhanced with intermediate list of pre-registered REACH substances
NEWS 8	NOV 21	CAS patent coverage to include exemplified prophetic substances identified in English-, French-, German-, and Japanese-language basic patents from 2004-present
NEWS 9	NOV 26	MARPAT enhanced with FSORT command
NEWS 10	NOV 26	MEDLINE year-end processing temporarily halts availability of new fully-indexed citations
NEWS 11	NOV 26	CHEMSAFE now available on STN Easy
NEWS 12	NOV 26	Two new SET commands increase convenience of STN searching
NEWS 13	DEC 01	ChemPort single article sales feature unavailable
NEWS 14	DEC 12	GBFULL now offers single source for full-text coverage of complete UK patent families

NEWS EXPRESS JUNE 27 08 CURRENT WINDOWS VERSION IS V8.3,
AND CURRENT DISCOVER FILE IS DATED 23 JUNE 2008.

NEWS HOURS	STN Operating Hours Plus Help Desk Availability
NEWS LOGIN	Welcome Banner and News Items
NEWS IPC8	For general information regarding STN implementation of IPC 8

Enter NEWS followed by the item number or name to see news on that specific topic.

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* * * * * * * * * * * * * * * * STN  Columbus  * * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 15:51:07 ON 12 DEC 2008

=> reg
THIS COMMAND NOT AVAILABLE IN THE CURRENT FILE
Some commands only work in certain files.  For example, the EXPAND
command can only be used to look at the index in a file which has an
index.  Enter "HELP COMMANDS" at an arrow prompt (=>) for a list of
commands which can be used in this file.

=> fil reg
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                       ENTRY    SESSION
FULL ESTIMATED COST                                     0.21       0.21

FILE 'REGISTRY' ENTERED AT 15:51:17 ON 12 DEC 2008
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
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Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES:   11 DEC 2008  HIGHEST RN 1083154-18-0
DICTIONARY FILE UPDATES:  11 DEC 2008  HIGHEST RN 1083154-18-0

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH July 5, 2008.

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document.  For information
on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

=>
Uploading C:\Program Files\Stnexp\Queries\10530646\Claim 8.str

L1      STRUCTURE UPLOADED

=> dis
L1 HAS NO ANSWERS
L1              STR
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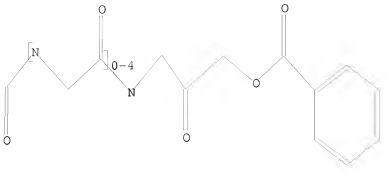

Structure attributes must be viewed using STN Express query preparation.

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=> s l1 sss full
FULL SEARCH INITIATED 15:51:40 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -    12060 TO ITERATE

100.0% PROCESSED    12060 ITERATIONS                                976 ANSWERS
SEARCH TIME: 00.00.01

L2          976 SEA SSS FUL L1

=> fil hcap
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                       ENTRY    SESSION
FULL ESTIMATED COST                                   178.36     178.57

FILE 'HCAPLUS' ENTERED AT 15:51:45 ON 12 DEC 2008
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
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FILE COVERS 1907 - 12 Dec 2008  VOL 149 ISS 25
FILE LAST UPDATED: 11 Dec 2008  (20081211/ED)

HCAplus now includes complete International Patent Classification (IPC)
reclassification data for the third quarter of 2008.

New CAS Information Use Policies, enter HELP USAGETERMS for details.
```

This file contains CAS Registry Numbers for easy and accurate substance identification.

```
=> l2
L3          164 L2

=> l3 and (pd<20050111)
      25919361 PD<20050111
                (PD<20050111)
L4          142 L3 AND (PD<20050111)

=> d l4 ibib abs hitstr 1-10
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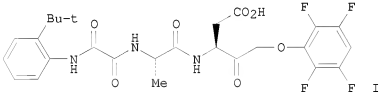
L4 ANSWER 1 OF 142 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER:	2005:1065682 HCAPLUS
DOCUMENT NUMBER:	143:432006
TITLE:	First-in-Class Pan Caspase Inhibitor Developed for the Treatment of Liver Disease
AUTHOR(S):	Linton, Steven D.; Aja, Teresa; Armstrong, Robert A.; Bai, Xu; Chen, Long-Shiuh; Chen, Ning; Ching, Brett; Contreras, Patricia; Diaz, Jose-Luis; Fisher, Craig D.; Fritz, Lawrence C.; Gladstone, Patricia; Groessl, Todd; Gu, Xin; Herrmann, Julia; Hirakawa, Brad P.; Hoglen, Niel C.; Jahangiri, Kathy G.; Kalish, Vincent J.; Karanewsky, Donald S.; Kodandapani, Lalitha; Krebs, Joseph; McQuiston, Jeff; Meduna, Steven P.; Nalley, Kip; Robinson, Edward D.; Sayers, Robert O.; Sebring, Kristen; Spada, Alfred P.; Ternansky, Robert J.; Tomaselli, Kevin J.; Ullman, Brett R.; Valentino, Karen L.; Weeks, Suzanne; Winn, David; Wu, Joe C.; Yeo, Pauline; Zhang, Cheng-zhi
CORPORATE SOURCE:	Idun Pharmaceuticals, San Diego, CA, 92121, USA
SOURCE:	Journal of Medicinal Chemistry (2005), 48(22), 6779-6782 CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER:	American Chemical Society
DOCUMENT TYPE:	Journal
LANGUAGE:	English
OTHER SOURCE(S):	CASREACT 143:432006

GI



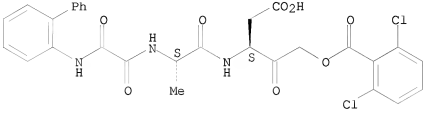
AB A series of oxamyl dipeptides were optimized for pan caspase inhibition, antiapoptotic cellular activity and in vivo efficacy. This structure-activity relationship study focused on the P4 oxamides and warhead moieties. Primarily on the basis of in vitro data, inhibitors

were selected for study in a murine model of α-Fas-induced liver injury. IDN-6556 (I) was further profiled in addnl. in vivo models and pharmacokinetic studies. This first-in-class caspase inhibitor is now the subject of two Phase II clin. trials, evaluating its safety and efficacy for use in liver disease.

IT 254749-48-9P 409367-56-2P 409367-61-9P
409367-77-7P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(first-in-class pan caspase inhibitor developed for treatment of liver disease)

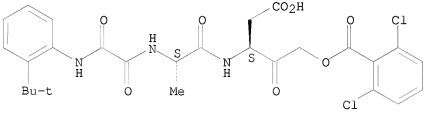
RN 254749-48-9 HCAPLUS
CN Benzoic acid, 2,6-dichloro-, (3S)-3-[[(2S)-2-[[2-([1,1'-biphenyl]-2-ylamino)-2-oxoacetyl]amino]-1-oxopropyl]amino]-4-carboxy-2-oxobutyl ester (CA INDEX NAME)

Absolute stereochemistry.



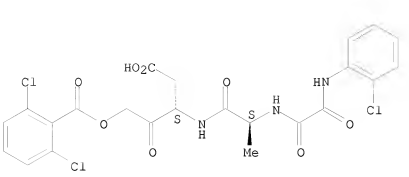
RN 409367-56-2 HCAPLUS
CN Benzoic acid, 2,6-dichloro-, (3S)-4-carboxy-3-[[(2S)-2-[[2-[[2-(1,1-dimethylethyl)phenyl]amino]-2-oxoacetyl]amino]-1-oxopropyl]amino]-2-oxobutyl ester (CA INDEX NAME)

Absolute stereochemistry.



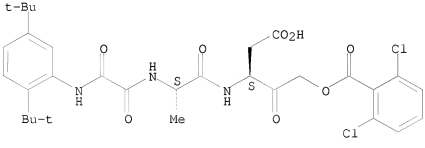
RN 409367-61-9 HCAPLUS
CN Benzoic acid, 2,6-dichloro-, (3S)-4-carboxy-3-[[(2S)-2-[[2-[(2-chlorophenyl)amino]-2-oxoacetyl]amino]-1-oxopropyl]amino]-2-oxobutyl ester (CA INDEX NAME)

Absolute stereochemistry.



RN 409367-77-7 HCAPLUS
CN Benzoic acid, 2,6-dichloro-, (3S)-3-[[(2S)-2-[[2-[[2,5-bis(1,1-dimethylethyl)phenyl]amino]-2-oxoacetyl]amino]-1-oxopropyl]amino]-4-carboxy-2-oxobutyl ester (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 44 THERE ARE 44 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 2 OF 142 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2005:1014174 HCAPLUS
DOCUMENT NUMBER: 143:452147
TITLE: Synthesis and evaluation of novel dipeptidyl benzoyloxymethyl ketones as caspase inhibitors
AUTHOR(S): Nedev, Hinyu N.; Klaiman, Guy; LeBlanc, Andrea; Saragovi, H. Uri
CORPORATE SOURCE: Department of Pharmacology and Therapeutics, Lady Davis Institute for Medical Research, McGill University, Jewish General Hospital, Montreal, QC, H3T 1E2, Can.
SOURCE: Biochemical and Biophysical Research Communications (2005), 336(2), 397-400
CODEN: BBRCA9; ISSN: 0006-291X
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 143:452147
AB We describe novel peptide-based caspase inhibitors. Potent and comparatively selective compds. containing a dipeptide scaffold and a substituted oxymethyl ketone as a warhead were developed. The newly

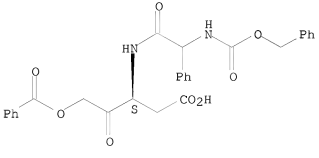
synthesized compds. were tested for inhibition in in vitro enzymic assays of caspases-1, -3, -6, -8, and -9. The benzyloxycarbonyl-phenylglycyl-aspartyl benzoyloxymethyl ketone (Z-Phg-Asp-CH2OCO-Ph, coded as HU44) was the most potent inhibitor of caspase-1 and caspase-3. Of several analogs of HU44 that were made, the β-Asp Me ester (2) is an effective inhibitor against caspase-3 and caspase-8, and less effective against caspase-1. These compds. did not inhibit caspase-6 and caspase-9 significantly.

IT 869117-83-9P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(synthesis and evaluation of dipeptidyl benzoyloxymethyl ketones as caspase inhibitors)

RN 869117-83-9 HCAPLUS

CN Pentanoic acid, 5-(benzoyloxy)-4-oxo-3-[[2-phenyl-2-[[(phenylmethoxy)carbonyl]amino]acetyl]amino]-, (3S)- (CA INDEX NAME)

Absolute stereochemistry.

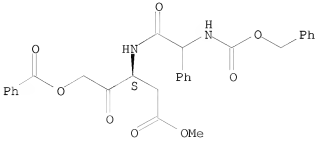


IT 869117-84-0 869117-86-2
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(synthesis and evaluation of dipeptidyl benzoyloxymethyl ketones as caspase inhibitors)

RN 869117-84-0 HCAPLUS

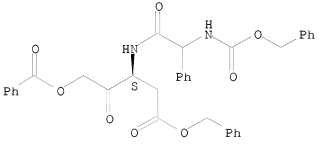
CN Pentanoic acid, 5-(benzoyloxy)-4-oxo-3-[[2-phenyl-2-[[(phenylmethoxy)carbonyl]amino]acetyl]amino]-, methyl ester, (3S)- (CA INDEX NAME)

Absolute stereochemistry.



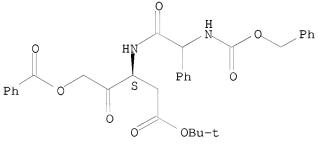
RN 869117-86-2 HCAPLUS
CN Pentanoic acid, 5-(benzoyloxy)-4-oxo-3-[[2-phenyl-2-[[(phenylmethoxy)carbonyl]amino]acetyl]amino]-, phenylmethyl ester, (3S)-
(CA INDEX NAME)

Absolute stereochemistry.



IT 869117-89-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(synthesis and evaluation of dipeptidyl benzoyloxymethyl ketones as caspase inhibitors)
RN 869117-89-5 HCAPLUS
CN Pentanoic acid, 5-(benzoyloxy)-4-oxo-3-[[2-phenyl-2-[[(phenylmethoxy)carbonyl]amino]acetyl]amino]-, 1,1-dimethylethyl ester, (3S)- (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 3 OF 142 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2005:864008 HCAPLUS
DOCUMENT NUMBER: 143:401965
TITLE: Dynamic imaging of protease activity with fluorescently quenched activity-based probes
AUTHOR(S): Blum, Galia; Mullins, Stefanie R.; Keren, Kinneret; Fonovic, Marko; Jedeszko, Christopher; Rice, Mark J.; Sloane, Bonnie F.; Bogyo, Matthew
CORPORATE SOURCE: Department of Pathology, Stanford University School of Medicine, Stanford, CA, 94305, USA

SOURCE: Nature Chemical Biology (2005), 1(4), 203-209
CODEN: NCBABT; ISSN: 1552-4450
PUBLISHER: Nature Publishing Group
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 143:401965

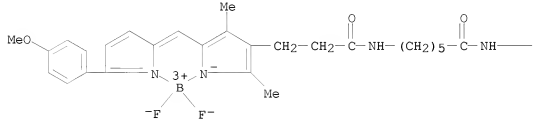
AB Protease activity is tightly regulated in both normal and disease conditions. However, it is often difficult to monitor the dynamic nature of this regulation in the context of a live cell or whole organism. To address this limitation, we developed a series of quenched activity-based probes (qABPs) that become fluorescent upon activity-dependent covalent modification of a protease target. These reagents freely penetrate cells and allow direct imaging of protease activity in living cells. Targeted proteases are directly identified and monitored biochem. by virtue of the resulting covalent tag, thereby allowing unambiguous assignment of protease activities observed in imaging studies. We report here the design and synthesis of a selective, cell-permeable qABP for the study of papain-family cysteine proteases. This probe is used to monitor real-time protease activity in live human cells with fluorescence microscopy techniques as well as standard biochem. methods.

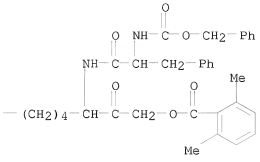
IT 867022-32-0P
RL: ARG (Analytical reagent use); SPN (Synthetic preparation); ANST (Analytical study); PREP (Preparation); USES (Uses)
(dynamic imaging of protease activity with fluorescently quenched activity-based probes)

RN 867022-32-0 HCAPLUS

CN Boron, difluoro[phenylmethyl (3S,6S)-6-[2-[(2,6-dimethylbenzoyl)oxy]acetyl]-21-[5-[[5-(4-methoxyphenyl)-2H-pyrrol-2-ylidene-κN]methyl]-2,4-dimethyl-1H-pyrrol-3-yl-κN]-4,12,19-trioxo-3-(phenylmethyl)-2,5,11,18-tetraazaheneicosanoato]-, (T-4)- (CA INDEX NAME)

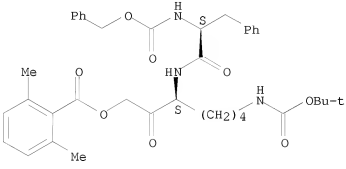
PAGE 1-A





IT 866951-92-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(dynamic imaging of protease activity with fluorescently quenched activity-based probes)
RN 866951-92-0 HCAPLUS
CN Benzoic acid, 2,6-dimethyl-, (3S)-7-[[(1,1-dimethylethoxy)carbonyl]amino]-2-oxo-3-[[(2S)-1-oxo-3-phenyl-2-[[(phenylmethoxy)carbonyl]amino]propyl]amino]heptyl ester (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 39 THERE ARE 39 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 4 OF 142 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2005:567513 HCAPLUS
DOCUMENT NUMBER: 143:262351
TITLE: Activity-based probes that target diverse cysteine protease families
AUTHOR(S): Kato, Daisuke; Boatright, Kelly M.; Berger, Alicia B.; Nazif, Tamim; Blum, Galia; Ryan, Ciara; Chehade, Kareem A. H.; Salvesen, Guy S.; Bogyo, Matthew
CORPORATE SOURCE: Department of Pathology, Stanford University School of Medicine, Stanford, CA, 940305, USA
SOURCE: Nature Chemical Biology (2005), 1(1), 33-38
CODEN: NCBABT; ISSN: 1552-4450
PUBLISHER: Nature Publishing Group

DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 143:262351

AB Proteases are one of the largest and best-characterized families of enzymes in the human proteome. Unfortunately, the understanding of protease function in the context of complex proteolytic cascades remains in its infancy. One major reason for this gap in understanding is the lack of technologies that allow direct assessment of protease activity. We report here an optimized solid-phase synthesis protocol that allows rapid generation of activity-based probes (ABPs) targeting a range of cysteine protease families. These reagents selectively form covalent bonds with the active-site thiol of a cysteine protease, allowing direct biochem. profiling of protease activities in complex proteomes. We present a number of probes containing either a single amino acid or an extended peptide sequence that target caspases, legumains, gingipains and cathepsins. Biochem. studies using these reagents highlight their overall utility and provide insight into the biochem. functions of members of these protease families.

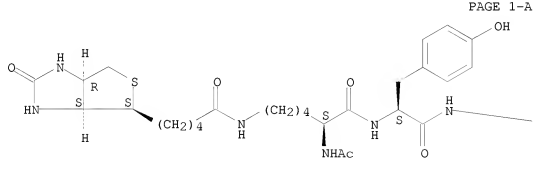
IT 863766-76-1P 863766-77-2P 863766-78-3P
863766-79-4P 863766-80-7P 863766-81-8P
863766-82-9P 863766-83-0P 863766-84-1P
863766-85-2P 863766-86-3P 863766-87-4P
RL: ARU (Analytical role, unclassified); BSU (Biological study, unclassified); BUU (Biological use, unclassified); SPN (Synthetic preparation); ANST (Analytical study); BIOL (Biological study); PREP (Preparation); USES (Uses)
(activity-based probes that target diverse cysteine protease families)

RN 863766-76-1 HCAPLUS

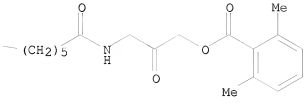
CN L-Tyrosinamide, N2-acetyl-N6-[5-[(3aS,4S,6aR)-hexahydro-2-oxo-1H-thieno[3,4-d]imidazol-4-yl]-1-oxopentyl]-L-lysyl-N-[6-[[3-[(2,6-dimethylbenzoyl)oxy]-2-oxopropyl]amino]-6-oxohexyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



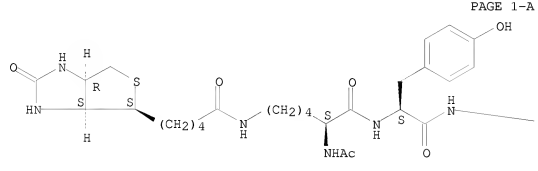
PAGE 1-B



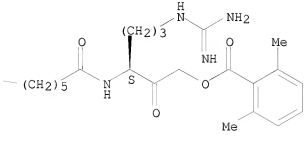
RN 863766-77-2 HCAPLUS
CN L-Tyrosinamide, N2-acetyl-N6-[5-[(3aS,4S,6aR)-hexahydro-2-oxo-1H-thieno[3,4-d]imidazol-4-yl]-1-oxopentyl]-L-lysyl-N-[6-[[(1S)-4-[(aminoiminomethyl)amino]-1-[[(2,6-dimethylbenzoyl)oxy]acetyl]butyl]amino]-6-oxohexyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



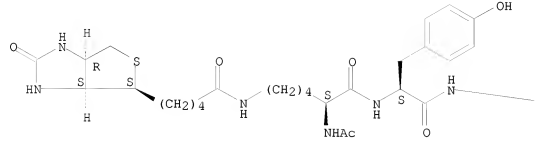
PAGE 1-B



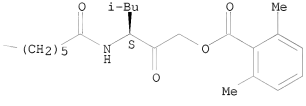
RN 863766-78-3 HCAPLUS
CN L-Tyrosinamide, N2-acetyl-N6-[5-[(3aS,4S,6aR)-hexahydro-2-oxo-1H-thieno[3,4-d]imidazol-4-yl]-1-oxopentyl]-L-lysyl-N-[6-[[(1S)-1-[[(2,6-dimethylbenzoyl)oxy]acetyl]-3-methylbutyl]amino]-6-oxohexyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



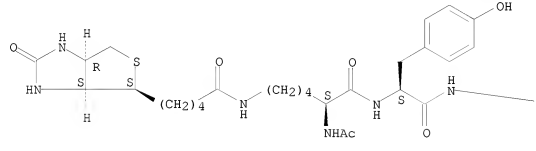
PAGE 1-B



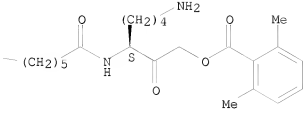
RN 863766-79-4 HCAPLUS
CN L-Tyrosinamide, N2-acetyl-N6-[5-[(3aS,4S,6aR)-hexahydro-2-oxo-1H-thieno[3,4-d]imidazol-4-yl]-1-oxopentyl]-L-lysyl-N-[6-[[(1S)-5-amino-1-[[(2,6-dimethylbenzoyl)oxy]acetyl]pentyl]amino]-6-oxohexyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



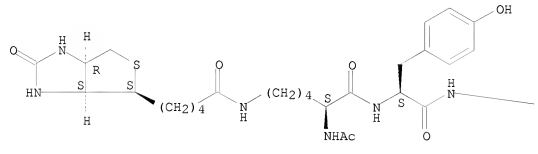
PAGE 1-B



RN 863766-80-7 HCAPLUS
CN L-Tyrosinamide, N2-acetyl-N6-[5-[(3aS,4S,6aR)-hexahydro-2-oxo-1H-thieno[3,4-d]imidazol-4-yl]-1-oxopentyl]-L-lysyl-N-[6-[[(1S)-1-(carboxymethyl)-3-[(2,6-dimethylbenzoyl)oxy]-2-oxopropyl]amino]-6-oxohexyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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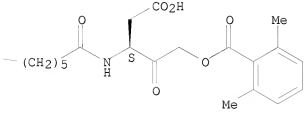
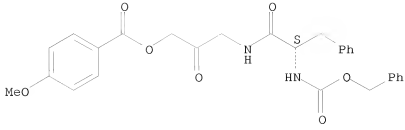


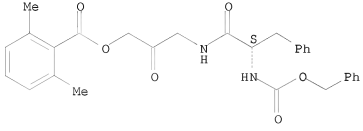
RN 863766-81-8 HCAPLUS
CN Benzoic acid, 4-methoxy-, 2-oxo-3-[[(2S)-1-oxo-3-phenyl-2-[[(phenylmethoxy)carbonyl]amino]propyl]amino]propyl ester (CA INDEX NAME)

Absolute stereochemistry.



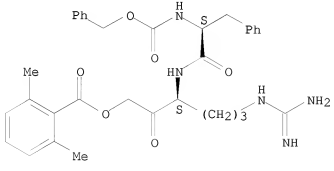
RN 863766-82-9 HCAPLUS
CN Benzoic acid, 2,6-dimethyl-, 2-oxo-3-[[(2S)-1-oxo-3-phenyl-2-[[(phenylmethoxy)carbonyl]amino]propyl]amino]propyl ester (CA INDEX NAME)

Absolute stereochemistry.



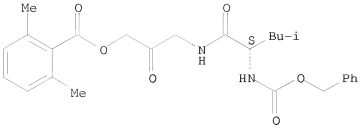
RN 863766-83-0 HCAPLUS
CN Benzoic acid, 2,6-dimethyl-, (3S)-6-[(aminoiminomethyl)amino]-2-oxo-3-[[(2S)-1-oxo-3-phenyl-2-[[(phenylmethoxy)carbonyl]amino]propyl]amino]hexyl ester (CA INDEX NAME)

Absolute stereochemistry.



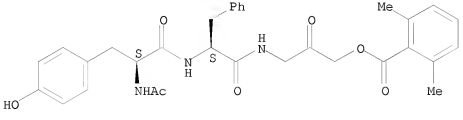
RN 863766-84-1 HCAPLUS
CN Benzoic acid, 2,6-dimethyl-, 3-[[(2S)-4-methyl-1-oxo-2-[[(phenylmethoxy)carbonyl]amino]pentyl]amino]-2-oxopropyl ester (CA INDEX NAME)

Absolute stereochemistry.



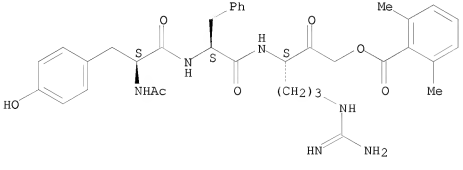
RN 863766-85-2 HCAPLUS
CN L-Phenylalaninamide, N-acetyl-L-tyrosyl-N-[3-[(2,6-dimethylbenzoyl)oxy]-2-oxopropyl]- (CA INDEX NAME)

Absolute stereochemistry.



RN 863766-86-3 HCAPLUS
CN L-Phenylalaninamide, N-acetyl-L-tyrosyl-N-[(1S)-4-[(aminoiminomethyl)amino]-1-[[(2,6-dimethylbenzoyl)oxy]acetyl]butyl]- (CA INDEX NAME)

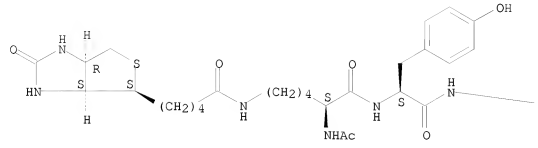
Absolute stereochemistry.



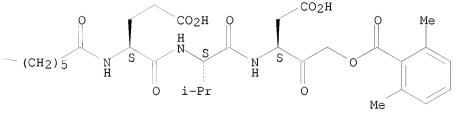
RN 863766-87-4 HCAPLUS
CN L-Valinamide, N2-acetyl-N6-[5-[(3aS,4S,6aR)-hexahydro-2-oxo-1H-thieno[3,4-d]imidazol-4-yl]-1-oxopentyl]-L-lysyl-L-tyrosyl-6-aminohexanoyl-L-α-glutamyl-N-[(1S)-1-(carboxymethyl)-3-[(2,6-dimethylbenzoyl)oxy]-2-oxopropyl]- (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

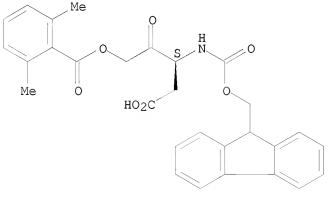


PAGE 1-B



IT 260434-73-9P 863766-65-8DP, resin bound
942347-28-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(activity-based probes that target diverse cysteine protease families)
RN 260434-73-9 HCAPLUS
CN Benzoic acid, 2,6-dimethyl-, (3S)-4-carboxy-3-[[(9H-fluoren-9-ylmethoxy)carbonyl]amino]-2-oxobutyl ester (CA INDEX NAME)

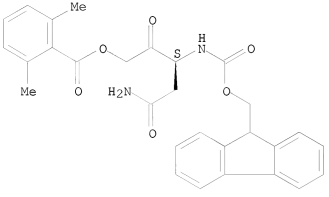
Absolute stereochemistry.



RN 863766-65-8 HCAPLUS

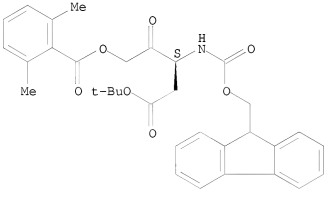
CN Benzoic acid, 2,6-dimethyl-, (3S)-5-amino-3-[[(9H-fluoren-9-ylmethoxy)carbonyl]amino]-2,5-dioxopentyl ester (CA INDEX NAME)

Absolute stereochemistry.



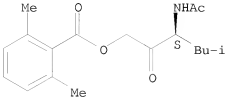
RN 942347-28-6 HCAPLUS
CN Benzoic acid, 2,6-dimethyl-, (3S)-5-(1,1-dimethylethoxy)-3-[[(9H-fluoren-9-ylmethoxy)carbonyl]amino]-2,5-dioxopentyl ester (CA INDEX NAME)

Absolute stereochemistry.



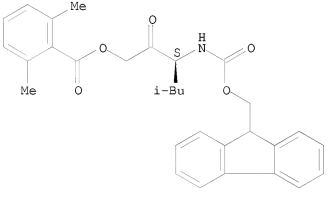
IT 863766-89-6P 863766-90-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(activity-based probes that target diverse cysteine protease families)
RN 863766-89-6 HCAPLUS
CN Benzoic acid, 2,6-dimethyl-, (3S)-3-(acetylamino)-5-methyl-2-oxohexyl ester (CA INDEX NAME)

Absolute stereochemistry.



RN 863766-90-9 HCAPLUS
CN Benzoic acid, 2,6-dimethyl-, (3S)-3-[[(9H-fluoren-9-ylmethoxy)carbonyl]amino]-5-methyl-2-oxohexyl ester (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 5 OF 142 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2005:557565 HCAPLUS
DOCUMENT NUMBER: 143:472445
TITLE: Neuroprotection by the caspase-1 inhibitor Ac-YVAD-(acyloxy)mk in experimental neuroAIDS is independent from IL-1β generation
AUTHOR(S): Corasaniti, M. T.; Russo, R.; Amantea, D.; Gliozzi, M.; Siviglia, E.; Stringaro, A. R.; Malorni, W.; Melino, G.; Bagetta, G.
CORPORATE SOURCE: Department of Pharmacobiological Sciences, University 'Magna Graecia' of Catanzaro, Catanzaro, Italy
SOURCE: Cell Death and Differentiation (2005), 12(Suppl. 1), 999-1001
CODEN: CDDIEK; ISSN: 1350-9047
PUBLISHER: Nature Publishing Group
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The HIV-1 gp120 elevates cytochrome c immunoreactivity into the cell cytoplasm of rat brain neocortex and this is an early event that occurs 6 h following a single intracerebral injection of the viral protein. Acetyl-Tyr-Val-Ala-Asp-2,6-dimethylbenzoyloxy-methylketone, an inhibitor of caspase-1, was able to counteract gp120-induced cytosolic cytochrome c

elevation and this without affecting IL-1β levels. Collectively, these observations suggest that Ac-YVAD-(acyloxy)mk prevents cytochrome c expression into the cytosol through a mechanism independent from inhibition of IL-1β generation.

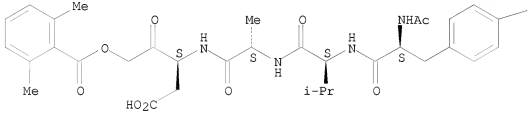
IT 154674-81-4
RL: DMA (Drug mechanism of action); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(caspase-1 inhibitor acetyl-Tyr-Val-Ala-Asp-2,6-dimethylbenzoyloxy-methylketone showed neuroprotection independent of interleukin-1β generation in neuroAIDS rat model)

RN 154674-81-4 HCAPLUS

CN L-Alaninamide, N-acetyl-L-tyrosyl-L-valyl-N-[(1S)-1-(carboxymethyl)-3-[(2,6-dimethylbenzoyl)oxy]-2-oxopropyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B

OH

REFERENCE COUNT: 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 6 OF 142 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2005:543231 HCAPLUS
DOCUMENT NUMBER: 144:186920
TITLE: Structural analysis of caspase-1 inhibitors derived from tethering
AUTHOR(S): O'Brien, Tom; Fahr, Bruce T.; Sopko, Michelle M.; Lam, Joni W.; Waal, Nathan D.; Raimundo, Brian C.; Purkey, Hans E.; Pham, Phuongly; Romanowski, Michael J.
CORPORATE SOURCE: Department of Biology, Sunesis Pharmaceuticals Inc., USA
SOURCE: Acta Crystallographica, Section F: Structural Biology and Crystallization Communications (2005), F61(5), 451-458
CODEN: ACSFCL; ISSN: 1744-3091
URL: http://journals.iucr.org/f/issues/2005/05/00/sx5030/sx5030.pdf
PUBLISHER: Blackwell Publishing Ltd.
DOCUMENT TYPE: Journal; (online computer file)
LANGUAGE: English

AB Caspase-1 is a key endopeptidase responsible for the post-translational processing of the IL-1β and IL-18 cytokines and small-mol. inhibitors

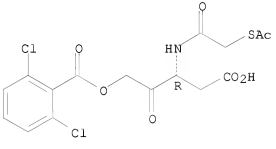
that modulate the activity of this enzyme are predicted to be important therapeutic treatments for many inflammatory diseases. A fragment-assembly approach, accompanied by structural anal., was employed to generate caspase-1 inhibitors. With the aid of Tethering with extenders (small mols. that bind to the active-site cysteine and contain a free thiol), two novel fragments that bound to the active site and made a disulfide bond with the extender were identified by mass spectrometry. Direct linking of each fragment to the extender generated submicromolar reversible inhibitors that significantly reduced secretion of IL-1β but not IL-6 from human peripheral blood mononuclear cells. Thus, Tethering with extenders facilitated rapid identification and synthesis of caspase-1 inhibitors with cell-based activity and subsequent structural analyses provided insights into the enzyme's ability to accommodate different inhibitor-binding modes in the active site.

IT 874985-07-6
RL: BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)
(structure-based fragment assembly process using Tethering with extenders for structural anal. of caspase-1 inhibitors that display cell-based activity)

RN 874985-07-6 HCAPLUS

CN Benzoic acid, 2,6-dichloro-, (3R)-3-[[2-(acetylthio)acetyl]amino]-4-carboxy-2-oxobutyl ester (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 38 THERE ARE 38 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 7 OF 142 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2005:157268 HCAPLUS

DOCUMENT NUMBER: 143:112404

TITLE: Delay of Iris flower senescence by protease inhibitors

AUTHOR(S): Pak, Caroline; van Doorn, Wouter G.

CORPORATE SOURCE: Agrotechnology and Food Innovations (A & F), Wageningen University and Research Centre, Wageningen, 6700 AA, Neth.

SOURCE: New Phytologist (2005), 165(2), 473-480
CODEN: NEPHAV; ISSN: 0028-646X

PUBLISHER: Blackwell Publishing Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Visible senescence of the flag tepals in Iris + hollandica (cv. Blue Magic) was preceded by a large increase in endoprotease activity. Just

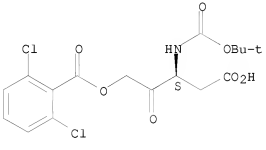
before visible senescence about half of total endoprotease activity was apparently due to cysteine proteases, somewhat less than half to serine proteases, with a minor role of metalloproteases. Treatment of isolated tepals with the purported serine protease inhibitors AEBSF [4-(2-aminoethyl)-benzenesulfonyl fluoride] or DFP (diisopropyl-fluorophosphate) prevented the increase in endoprotease activity and considerably delayed or prevented the normal senescence symptoms. The specific cysteine protease-specific E-64d reduced maximum endoprotease activity by 30%, but had no effect on the time to visible senescence. Zinc chloride and aprotinin reduced maximum endoprotease activity by c. 50 and 40%, resp., and slightly delayed visible senescence. A proteasome inhibitor (Z-leu-leu-Nva-H) slightly delayed tepal senescence, which indicates that protein degradation in the proteasome may play a role in induction of the visible senescence symptoms. Thus, visible senescence is preceded by large-scale protein degradation, which is apparently mainly due to cysteine- and serine protease activity, and two (unspecific) inhibitors of serine proteases considerably delay the senescence symptoms.

IT 857895-08-0
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(Iris flower senescence delay by protease inhibitors)

RN 857895-08-0 HCAPLUS

CN Benzoic acid, 2,6-dichloro-, (3S)-4-carboxy-3-[[(1,1-dimethylethoxy)carbonyl]amino]-2-oxobutyl ester (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 47 THERE ARE 47 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 8 OF 142 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2005:130294 HCAPLUS

DOCUMENT NUMBER: 142:392641

TITLE: Dipeptidyl aspartyl fluoromethylketones as potent caspase inhibitors: peptidomimetic replacement of the P2 α-amino acid by a α-hydroxy acid

AUTHOR(S): Wang, Yan; Guan, Lufeng; Jia, Shaojuan; Tseng, Ben; Drewe, John; Cai, Sui Xiong

CORPORATE SOURCE: Maxim Pharmaceuticals, San Diego, CA, 92121, USA

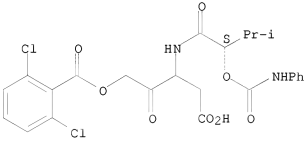
SOURCE: Bioorganic & Medicinal Chemistry Letters (2005), 15(5), 1379-1383
CODEN: BMCLE8; ISSN: 0960-894X

PUBLISHER: Elsevier B.V.

DOCUMENT TYPE: Journal

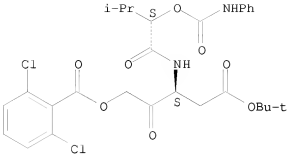
LANGUAGE: English
OTHER SOURCE(S): CASREACT 142:392641
AB As a continuation of our SAR (structure activity relationship) studies of dipeptidyl asparty1-fmk as caspase inhibitors, we explored the replacement of the P2 α-amino acid by a peptidomimetic α-hydroxy acid. These α-carbamoyl-alkylcarbonyl-aspartyl fluoromethylketones were found to be potent caspase inhibitors, and the SAR of these compds. is similar to the corresponding dipeptidyl asparty1-fmk. MX1153, (S)-3-methyl-2-(phenylcarbamoyl)butanoyl-Asp-fmk, is identified as a potent broad-spectrum caspase inhibitor, and is selective for caspases vs. other proteases. MX1153 also has good activity in the cell apoptosis protection assays and is active in the mouse liver apoptosis model.
IT 582317-45-1P
RL: BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation and structure-activity relationship of dipeptidyl aspartyl fluoromethylketones as potent caspase inhibitors)
RN 582317-45-1 HCAPLUS
CN Benzoic acid, 2,6-dichloro-, 4-carboxy-3-[[(2S)-3-methyl-1-oxo-2-[[(phenylamino)carbonyl]oxy]butyl]amino]-2-oxobutyl ester (CA INDEX NAME)

Absolute stereochemistry.



IT 329046-55-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and structure-activity relationship of dipeptidyl aspartyl fluoromethylketones as potent caspase inhibitors)
RN 329046-55-1 HCAPLUS
CN Benzoic acid, 2,6-dichloro-, (3S)-5-(1,1-dimethylethoxy)-3-[[(2S)-3-methyl-1-oxo-2-[[(phenylamino)carbonyl]oxy]butyl]amino]-2,5-dioxopentyl ester (CA INDEX NAME)

Absolute stereochemistry.

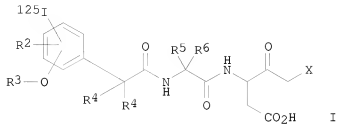


REFERENCE COUNT: 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 9 OF 142 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2004:675705 HCAPLUS
DOCUMENT NUMBER: 141:207524
TITLE: Preparation of peptidyl irreversible caspase-3 inhibitors as active site probes
INVENTOR(S): Colucci, John; Giroux, Andre; Han, Yongxin; Methot, Nathalie; Nicholson, Donald W.; Roy, Sophie; Vaillancourt, John Paul; Tawa, Paul
PATENT ASSIGNEE(S): Merck Frosst Canada & Co., Can.
SOURCE: PCT Int. Appl., 70 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004069773	A1	20040819	WO 2004-CA152	20040205 <--
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI				
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2514441	A1	20041019	CA 2004-2514441	20040205 <--
EP 1594819	A1	20051116	EP 2004-708291	20040205
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
JP 2006519777	T	20060831	JP 2006-501408	20040205
US 20060069038	A1	20060330	US 2005-542684	20050719
PRIORITY APPLN. INFO.:			US 2003-445560P P	20030207
			WO 2004-CA152 W	20040205

OTHER SOURCE(S): MARPAT 141:207524
GI



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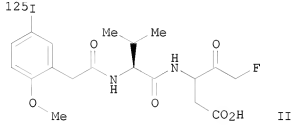


II

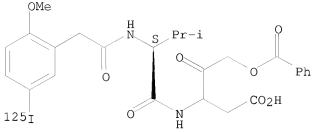
AB The invention encompasses compds. I [X is halo or O-W-Z, where W is a bond, CH2, CO or COCH2 and Z is H, alkyl, cycloalkyl, Ph, etc.; R2 is H, halo, hydroxy, nitro, cyano, alkyl, etc.; R3 is Ph or (un)substituted alkyl; R4 is H, halo, hydroxy, (un)substituted alkyl or alkoxy; R5 is H, Ph, naphthyl, (un)substituted alkyl or cycloalkyl and R6 is H or R5 and R6 together form a ring] which are useful for determining whether a caspase has been activated in cells or in tissues of animal models of various pathologies. Furthermore, through competition based assays, these caspase active site probes can be used to calculate the percentage of occupancy of active caspases by other, unlabeled inhibitors. Thus, peptide II was prepared via coupling reactions of Me (5-iodo-2-methoxyphenyl)acetate, L-valine tert-Bu ester hydrochloride, and tert-Bu 3-amino-2,3,5-trideoxy-5-fluoropentonate, followed by tributylstannylation, iodination, and deprotection with TFA. II was assayed for inhibition of a subset of caspases and for detection of active caspases in protein exts.

IT 741293-00-5P 741293-01-6P 741293-02-7P
RL: DGN (Diagnostic use); PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of peptidyl irreversible caspase-3 inhibitors as active site probes)

RN 741293-00-5 HCAPLUS

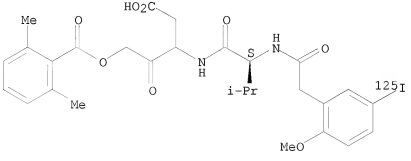
CN Pentanoic acid, 5-(benzoyloxy)-3-[[(2S)-2-[[[5-(iodo-125I)-2-methoxyphenyl]acetyl]amino]-3-methyl-1-oxobutyl]amino]-4-oxo- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



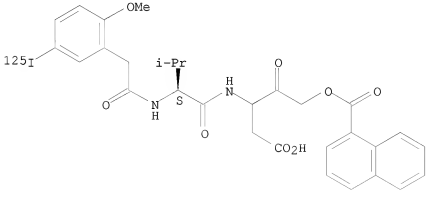
RN 741293-01-6 HCAPLUS
CN Benzoic acid, 2,6-dimethyl-, 4-carboxy-3-[[(2S)-2-[[[5-(iodo-125I)-2-methoxyphenyl]acetyl]amino]-3-methyl-1-oxobutyl]amino]-2-oxobutyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 741293-02-7 HCAPLUS
CN 1-Naphthalenecarboxylic acid, 4-carboxy-3-[[(2S)-2-[[[5-(iodo-125I)-2-methoxyphenyl]acetyl]amino]-3-methyl-1-oxobutyl]amino]-2-oxobutyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L4 ANSWER 10 OF 142 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2004:606353 HCAPLUS
DOCUMENT NUMBER: 141:151000
TITLE: Methods for reducing mortality associated with acute myocardial infarction
INVENTOR(S): Bell, Leonard
PATENT ASSIGNEE(S): Alexion Pharmaceuticals, Inc., USA
SOURCE: PCT Int. Appl., 31 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004062578	A2	20040729	WO 2004-US1189	20040106 <--
WO 2004062578	A3	20051013		
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US 20040219147	A1	20041104	US 2003-339562	20030109 <--
US 7361339	B2	20080422		
AU 2004204834	A1	20040729	AU 2004-204834	20040106 <--
AU 2004204834	B2	20080828		
CA 2511659	A1	20040729	CA 2004-2511659	20040106 <--
EP 1592383	A2	20051109	EP 2004-700408	20040106
EP 1592383	A3	20051207		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
JP 2006516978	T	20060713	JP 2006-500995	20040106

PRIORITY APPLN. INFO.:
US 2003-339562 A 20030109
WO 2004-US1189 W 20040106

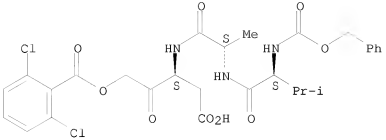
AB Methods of reducing mortality in myocardial infarction patients receiving a stent in connection with percutaneous transluminal coronary angioplasty include administering an anti-inflammatory compound to the patient. In one embodiment, the anti-inflammatory compound is an antibody-to a complement component.

IT 151594-01-3 153088-73-4
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(methods for reducing mortality associated with acute myocardial infarction using an antiinflammatory agent)

RN 151594-01-3 HCAPLUS

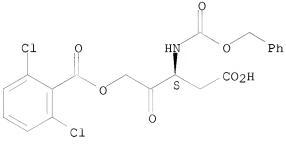
CN L-Alaninamide, N-[(phenylmethoxy)carbonyl]-L-valyl-N-[(1S)-1-(carboxymethyl)-3-[(2,6-dichlorobenzoyl)oxy]-2-oxopropyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 153088-73-4 HCAPLUS
CN Benzoic acid, 2,6-dichloro-, (3S)-4-carboxy-2-oxo-3-[[(phenylmethoxy)carbonyl]amino]butyl ester (CA INDEX NAME)

Absolute stereochemistry.



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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 11 DEC 2008 HIGHEST RN 1083154-18-0
DICTIONARY FILE UPDATES: 11 DEC 2008 HIGHEST RN 1083154-18-0

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH July 5, 2008.

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  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

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predicted properties as well as tags indicating availability of
experimental property data in the original document.  For information
on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

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*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

Structure attributes must be viewed using STN Express query preparation.


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FULL SCREEN SEARCH COMPLETED -     8087 TO ITERATE

100.0% PROCESSED     8087 ITERATIONS                              13 ANSWERS
SEARCH TIME: 00.00.01

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CA SUBSCRIBER PRICE                                   0.00      -8.00

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FILE COVERS 1907 - 12 Dec 2008  VOL 149 ISS 25
FILE LAST UPDATED: 11 Dec 2008  (20081211/ED)

HCAplus now includes complete International Patent Classification (IPC)
reclassification data for the third quarter of 2008.

New CAS Information Use Policies, enter HELP USAGETERMS for details.

 This file contains CAS Registry Numbers for easy and accurate
 substance identification.

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L7            1 L6

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L7   ANSWER 1 OF 1  HCAPLUS  COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER:         2004:333680  HCAPLUS
DOCUMENT NUMBER:          140:357669
TITLE:                    Preparation of peptidyl activity-based probes for
                          catalytically-active enzymes
INVENTOR(S):              Winn, David; Campbell, David Alan
PATENT ASSIGNEE(S):       Activx Biosciences, Inc., USA
SOURCE:                   PCT Int. Appl., 61 pp.
                          CODEN: PIXXD2
DOCUMENT TYPE:            Patent
LANGUAGE:                 English
FAMILY ACC. NUM. COUNT:   1
PATENT INFORMATION:

     PATENT NO.          KIND   DATE        APPLICATION NO.         DATE
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     WO 2004033397        A2    20040422    WO 2003-US32152         20031008
     WO 2004033397        A3    20060727
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             GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK,
             LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ,
             OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM,
             TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
         RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
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             BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
     CA 2501831           A1    20040422    CA 2003-2501831         20031008
     AU 2003282575        A1    20040504    AU 2003-282575          20031008
     EP 1583726           A2    20051012    EP 2003-774762          20031008
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     JP 2006514824        T     20060518    JP 2004-543659          20031008
     US 20070141624       A1    20070621    US 2006-530646          20060111
PRIORITY APPLN. INFO.:                      US 2002-417664P     P   20021009
                                            WO 2003-US32152     W   20031008
OTHER SOURCE(S):          MARPAT 140:357669
AB   The invention provides compns. and methods for assessing profiles of
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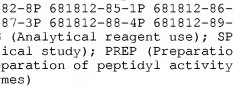
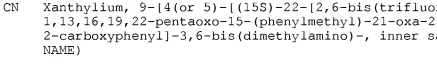
catalytically-active enzymes (e.g., a hydrolase, most preferably a cysteine protease) in compns. containing a plurality of proteins. The methods use activity-based probes (ABPs) that have an affinity moiety for directing the binding of the ABP to one or more catalytically-active target enzymes, a reactive group for forming a covalent bond at an active site of the target enzyme(s), and a TAG (e.g., a detectable label, preferably a fluorophore). ABPs TAG-L-CO(NHCHR2CO)nNHCHR1-RG [R1, R2 are H, alkyl optionally containing 1-3 heteroatoms N, O, or S, alkylaryl, -heteroaryl, or -phenyl; RG is a reactive group that reacts to form a covalent bond with a catalytically-active target enzyme; L is optionally present and is an alkyl or heteroalkyl group of 1-20 backbone atoms selected from NR, O, S or CR2, where R is H or alkyl; n is 1-4] or pharmaceutically-acceptable salts or complexes are claimed. One or more ABPs may be combined with a protein-containing sample under conditions for binding and reaction of the ABP(s) with target enzyme(s) that are present in the sample. The resulting products may then be used to assess the active enzyme profile of the sample and can be correlated to the presence, amount, or activity of one or more target enzyme(s) present in the original complex protein mixture An example describes the synthesis of ANP TAMRA-NH(CH2)10CO-L-Asp-CH2OC6HF4-2,3,5,6, where TAMRA is a rhodamine dye.

IT 681812-82-8P 681812-85-1P 681812-86-2P
681812-87-3P 681812-88-4P 681812-89-5P
RL: ARG (Analytical reagent use); SPN (Synthetic preparation); ANST (Analytical study); PREP (Preparation); USES (Uses)
(preparation of peptidyl activity-based probes for catalytically-active enzymes)

RN 681812-82-8 HCAPLUS

CN Xanthylium, 9-[4(or 5)-[(15S)-22-[2,6-bis(trifluoromethyl)phenyl]-1,13,16,19,22-pentaoxo-15-(phenylmethyl)-21-oxa-2,14,17-triazadocos-1-yl]-2-carboxyphenyl]-3,6-bis(dimethylamino)-, inner salt (9CI) (CA INDEX NAME)

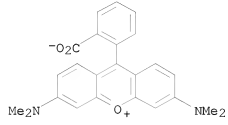


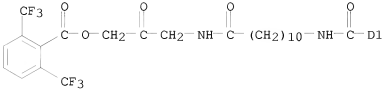


RN 681812-85-1 HCAPLUS

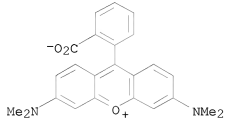
CN Xanthylium, 9-[4(or 5)-[[[11-[[3-[[2,6-bis(trifluoromethyl)benzoyl]oxy]-2-

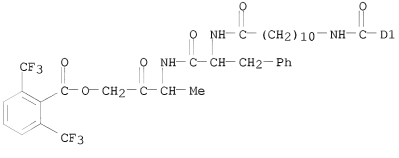
oxopropyl]amino]-11-oxoundecyl]amino]carbonyl]-2-carboxyphenyl]-3,6-bis(dimethylamino)-, inner salt (9CI) (CA INDEX NAME)





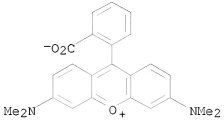
RN 681812-86-2 HCAPLUS
CN Xanthylium, 9-[4(or 5)-[(15S,18S)-22-[2,6-bis(trifluoromethyl)phenyl]-18-methyl-1,13,16,19,22-pentaoxo-15-(phenylmethyl)-21-oxa-2,14,17-triazadocos-1-yl]-2-carboxyphenyl]-3,6-bis(dimethylamino)-, inner salt (9CI) (CA INDEX NAME)

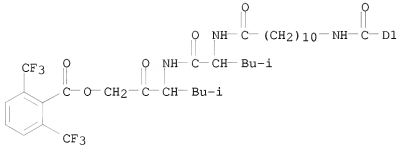




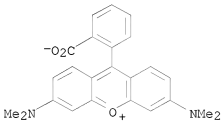
RN 681812-87-3 HCAPLUS
CN Xanthylium, 9-[4(or 5)-[(15S,18S)-22-[2,6-bis(trifluoromethyl)phenyl]-15,18-bis(2-methylpropyl)-1,13,16,19,22-pentaoxo-21-oxa-2,14,17-

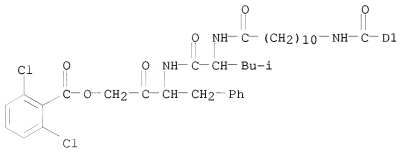
triazadocos-1-yl]-2-carboxyphenyl]-3,6-bis(dimethylamino)-, inner salt (9CI) (CA INDEX NAME)



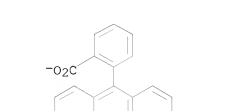


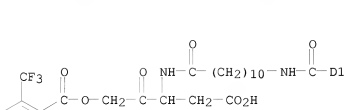
RN 681812-88-4 HCAPLUS
CN Xanthylium, 9-[2-carboxy-4(or 5)-[(15S,18S)-22-(2,6-dichlorophenyl)-15-(2-methylpropyl)-1,13,16,19,22-pentaoxo-18-(phenylmethyl)-21-oxa-2,14,17-triazadocos-1-yl]phenyl]-3,6-bis(dimethylamino)-, inner salt (9CI) (CA INDEX NAME)





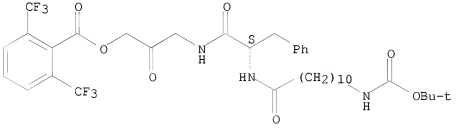
RN 681812-89-5 HCAPLUS
CN Xanthylium, 9-[4(or 5)-[[[11-[[(1S)-3-[[2,6-bis(trifluoromethyl)benzoyl]oxy]-1-(carboxymethyl)-2-oxopropyl]amino]-11-oxoundecyl]amino]carbonyl]-2-carboxyphenyl]-3,6-bis(dimethylamino)-, inner salt (9CI) (CA INDEX NAME)





IT 681447-89-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of peptidyl activity-based probes for catalytically-active enzymes)
RN 681447-89-2 HCAPLUS
CN Benzoic acid, 2,6-bis(trifluoromethyl)-, (6S)-22,22-dimethyl-2,5,8,20-tetraoxo-6-(phenylmethyl)-21-oxa-4,7,19-triazatricos-1-yl ester (CA INDEX NAME)

Absolute stereochemistry.



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COST IN U.S. DOLLARS SINCE FILE ENTRY TOTAL SESSION

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FULL ESTIMATED COST                                    21.59     457.23

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)       SINCE FILE      TOTAL
                                                    ENTRY    SESSION
CA SUBSCRIBER PRICE                                 -0.80      -8.80

FILE 'REGISTRY' ENTERED AT 16:01:35 ON 12 DEC 2008
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provided by InfoChem.

STRUCTURE FILE UPDATES:   11 DEC 2008  HIGHEST RN 1083154-18-0
DICTIONARY FILE UPDATES:  11 DEC 2008  HIGHEST RN 1083154-18-0

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH July 5, 2008.

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document.  For information
on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

=>
Uploading C:\Program Files\Stnexp\Queries\10530646\Claim 1 Compound 1.str

L8      STRUCTURE UPLOADED

=> dis
L8 HAS NO ANSWERS
L8              STR
*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

Structure attributes must be viewed using STN Express query preparation.


=> s l8 sss full
FULL SEARCH INITIATED 16:05:31 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -     8274 TO ITERATE

100.0% PROCESSED     8274 ITERATIONS                                 7 ANSWERS
SEARCH TIME: 00.00.01

L9            7 SEA SSS FUL L8

=> hcap
L10          31 HCAP
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COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                      ENTRY    SESSION
FULL ESTIMATED COST                                   186.27     643.50

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)          SINCE FILE      TOTAL
                                                      ENTRY    SESSION
CA SUBSCRIBER PRICE                                     0.00      -8.80

FILE 'HCAPLUS' ENTERED AT 16:05:45 ON 12 DEC 2008
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FILE COVERS 1907 - 12 Dec 2008  VOL 149 ISS 25
FILE LAST UPDATED: 11 Dec 2008  (20081211/ED)

HCAplus now includes complete International Patent Classification (IPC)
reclassification data for the third quarter of 2008.

New CAS Information Use Policies, enter HELP USAGETERMS for details.

 This file contains CAS Registry Numbers for easy and accurate
 substance identification.

=> l9
L11           1 L9

=> d l11

L11  ANSWER 1 OF 1  HCAPLUS  COPYRIGHT 2008 ACS on STN
AN   2004:333680  HCAPLUS
DN   140:357669
TI   Preparation of peptidyl activity-based probes for catalytically-active
     enzymes
IN   Winn, David; Campbell, David Alan
PA   Activx Biosciences, Inc., USA
SO   PCT Int. Appl., 61 pp.
     CODEN: PIXXD2
DT   Patent
LA   English
FAN.CNT 1
     PATENT NO.          KIND   DATE        APPLICATION NO.        DATE
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PI   WO 2004033397        A2    20040422    WO 2003-US32152        20031008
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     WO 2004033397        A3    20060727
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             CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE,
             GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK,
             LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ,
             OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM,
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             FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR,
             BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
     CA 2501831           A1    20040422    CA 2003-2501831         20031008
     AU 2003282575        A1    20040504    AU 2003-282575          20031008
     EP 1583726           A2    20051012    EP 2003-774762          20031008
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     JP 2006514824        T     20060518    JP 2004-543659          20031008
     US 20070141624       A1    20070621    US 2006-530646          20060111
PRAI US 2002-417664P      P     20021009
     WO 2003-US32152      W     20031008
OS   MARPAT 140:357669


=> d L11 ibib abs hitstr

L11  ANSWER 1 OF 1  HCAPLUS  COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER:         2004:333680  HCAPLUS
DOCUMENT NUMBER:          140:357669
TITLE:                    Preparation of peptidyl activity-based probes for
                          catalytically-active enzymes
INVENTOR(S):              Winn, David; Campbell, David Alan
PATENT ASSIGNEE(S):       Activx Biosciences, Inc., USA
SOURCE:                   PCT Int. Appl., 61 pp.
                          CODEN: PIXXD2
DOCUMENT TYPE:            Patent
LANGUAGE:                 English
FAMILY ACC. NUM. COUNT:   1
PATENT INFORMATION:

     PATENT NO.           KIND   DATE        APPLICATION NO.         DATE
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     WO 2004033397         A2    20040422    WO 2003-US32152         20031008
     WO 2004033397         A3    20060727
         W:  AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
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             GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK,
             LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ,
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             TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
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             KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES,
             FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR,
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     CA 2501831            A1    20040422    CA 2003-2501831         20031008
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     EP 1583726            A2    20051012    EP 2003-774762          20031008
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R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK

JP 2006514824	T	20060518	JP 2004-543659		20031008
US 20070141624	A1	20070621	US 2006-530646		20060111
PRIORITY APPLN. INFO.:			US 2002-417664P	P	20021009
			WO 2003-US32152	W	20031008

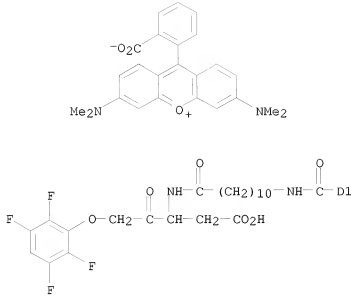
OTHER SOURCE(S): MARPAT 140:357669

AB The invention provides compns. and methods for assessing profiles of catalytically-active enzymes (e.g., a hydrolase, most preferably a cysteine protease) in compns. containing a plurality of proteins. The methods use activity-based probes (ABPs) that have an affinity moiety for directing the binding of the ABP to one or more catalytically-active target enzymes, a reactive group for forming a covalent bond at an active site of the target enzyme(s), and a TAG (e.g., a detectable label, preferably a fluorophore). ABPs TAG-L-CO(NHCHR2CO)nNHCHR1-RG [R1, R2 are H, alkyl optionally containing 1-3 heteroatoms N, O, or S, alkylaryl, -heteroaryl, or -phenyl; RG is a reactive group that reacts to form a covalent bond with a catalytically-active target enzyme; L is optionally present and is an alkyl or heteroalkyl group of 1-20 backbone atoms selected from NR, O, S or CR2, where R is H or alkyl; n is 1-4] or pharmaceutically-acceptable salts or complexes are claimed. One or more ABPs may be combined with a protein-containing sample under conditions for binding and reaction of the ABP(s) with target enzyme(s) that are present in the sample. The resulting products may then be used to assess the active enzyme profile of the sample and can be correlated to the presence, amount, or activity of one or more target enzyme(s) present in the original complex protein mixture An example describes the synthesis of ANP TAMRA-NH(CH2)10CO-L-Asp-CH2OC6HF4-2,3,5,6, where TAMRA is a rhodamine dye.

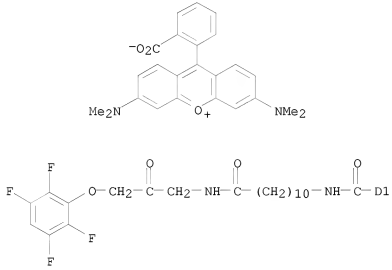
IT 681812-81-7P 681812-83-9P 681812-84-0P
RL: ARG (Analytical reagent use); SPN (Synthetic preparation); ANST (Analytical study); PREP (Preparation); USES (Uses)
(preparation of peptidyl activity-based probes for catalytically-active enzymes)

RN 681812-81-7 HCAPLUS

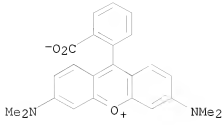
CN Xanthylium, 9-[2-carboxy-4(or 5)-[[[11-[[(1S)-1-(carboxymethyl)-2-oxo-3-(2,3,5,6-tetrafluorophenoxy)propyl]amino]-11-oxoundecyl]amino]carbonyl]phenyl]-3,6-bis(dimethylamino)-, inner salt (9CI) (CA INDEX NAME)

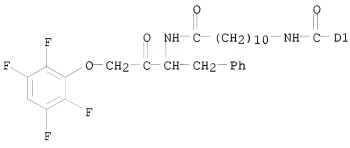


RN 681812-83-9 HCAPLUS
CN Xanthylium, 9-[2-carboxy-4(or 5)-[[[11-oxo-11-[[2-oxo-3-(2,3,5,6-tetrafluorophenoxy)propyl]amino]undecyl]amino]carbonyl]phenyl]-3,6-bis(dimethylamino)-, inner salt (9CI) (CA INDEX NAME)



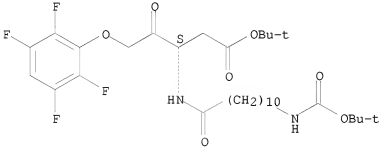
RN 681812-84-0 HCAPLUS
CN Xanthylium, 9-[2-carboxy-4(or 5)-[[[11-oxo-11-[[(1S)-2-oxo-1-(phenylmethyl)-3-(2,3,5,6-tetrafluorophenoxy)propyl]amino]undecyl]amino]carbonyl]phenyl]-3,6-bis(dimethylamino)-, inner salt (9CI) (CA INDEX NAME)





IT 681447-86-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of peptidyl activity-based probes for catalytically-active enzymes)
RN 681447-86-9 HCAPLUS
CN Pentanoic acid, 3-[[11-[[(1,1-dimethylethoxy)carbonyl]amino]-1-oxoundecyl]amino]-4-oxo-5-(2,3,5,6-tetrafluorophenoxy)-, 1,1-dimethylethyl ester, (3S)- (CA INDEX NAME)

Absolute stereochemistry.



=> d que stat
L8 STR

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

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Structure attributes must be viewed using STN Express query preparation.
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L11            1 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L9


=> d his full

     (FILE 'HOME' ENTERED AT 15:51:07 ON 12 DEC 2008)

     FILE 'REGISTRY' ENTERED AT 15:51:17 ON 12 DEC 2008
L1                 STRUCTURE UPLOADED
                   DIS
L2           976 SEA SSS FUL L1

     FILE 'HCAPLUS' ENTERED AT 15:51:45 ON 12 DEC 2008
L3           164 SEA ABB=ON  PLU=ON  L2
L4           142 SEA ABB=ON  PLU=ON  L3 AND (PD<20050111)
                   D L4 IBIB ABS HITSTR 1-10

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L5                 STRUCTURE UPLOADED
                   DIS
L6            13 SEA SSS FUL L5

     FILE 'HCAPLUS' ENTERED AT 15:57:52 ON 12 DEC 2008
L7             1 SEA ABB=ON  PLU=ON  L6
                   D L7 IBIB ABS HITSTR

     FILE 'REGISTRY' ENTERED AT 16:01:35 ON 12 DEC 2008
L8                 STRUCTURE UPLOADED
                   DIS
L9             7 SEA SSS FUL L8
L10           31 SEA ABB=ON  PLU=ON  HCAP

     FILE 'HCAPLUS' ENTERED AT 16:05:45 ON 12 DEC 2008
L11            1 SEA ABB=ON  PLU=ON  L9
                   D L11
                   D L11 IBIB ABS HITSTR
                   D QUE STAT


     FILE HOME

     FILE REGISTRY
     Property values tagged with IC are from the ZIC/VINITI data file
     provided by InfoChem.

     STRUCTURE FILE UPDATES:   11 DEC 2008  HIGHEST RN 1083154-18-0
     DICTIONARY FILE UPDATES:  11 DEC 2008  HIGHEST RN 1083154-18-0

     New CAS Information Use Policies, enter HELP USAGETERMS for details.

     TSCA INFORMATION NOW CURRENT THROUGH July 5, 2008.

       Please note that search-term pricing does apply when
       conducting SmartSELECT searches.
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REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

FILE HCAPLUS

FILE COVERS 1907 - 12 Dec 2008 VOL 149 ISS 25
FILE LAST UPDATED: 11 Dec 2008 (20081211/ED)

HCAplus now includes complete International Patent Classification (IPC) reclassification data for the third quarter of 2008.

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.